



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 1KS9 / pdb_00001ks9
Title : Ketopantoate Reductase from Escherichia coli
Authors : Matak-Vinkovic, D.; Vinkovic, M.; Saldanha, S.A.; Ashurst, J.A.; von Delft, F.; Inoue, T.; Miguel, R.N.; Smith, A.G.; Blundell, T.L.; Abell, C.
Deposited on : 2002-01-11
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

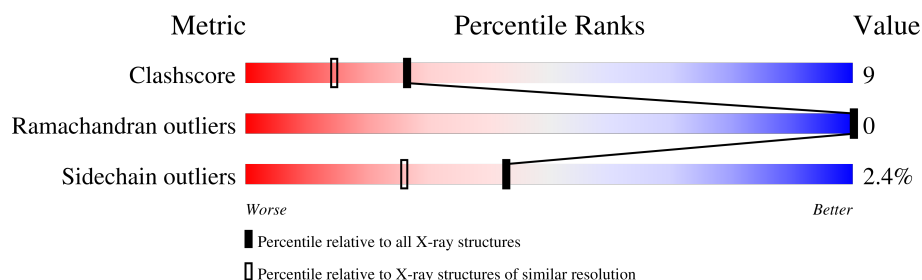
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	291	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-DEHYDROPANTOATE 2-REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2267	1424	402	428	13			

- Molecule 2 is water.

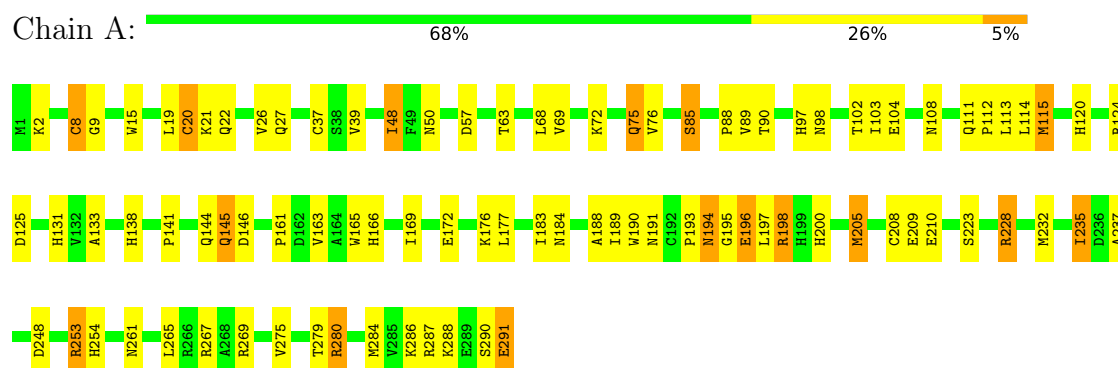
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	265	Total	O	0	0
			265	265		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 2-DEHYDROPANTOATE 2-REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.73Å 103.73Å 55.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2532	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	1/2310 (0.0%)	2.14	91/3148 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLN	N-CA	-5.61	1.38	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	CYS	CA-C-O	-21.95	94.72	119.97
1	A	48	ILE	CA-C-O	-20.95	98.46	121.93
1	A	20	CYS	O-C-N	14.50	140.11	122.27
1	A	48	ILE	O-C-N	13.12	138.10	122.36
1	A	21	LYS	CA-C-N	10.98	142.26	122.38
1	A	21	LYS	C-N-CA	10.98	142.26	122.38
1	A	197	LEU	CA-C-O	-10.86	107.83	120.10
1	A	196	GLU	CA-C-O	9.12	130.22	120.55
1	A	115	MET	N-CA-CB	-9.11	95.51	111.08
1	A	197	LEU	O-C-N	9.09	132.85	122.22
1	A	27	GLN	OE1-CD-NE2	9.05	131.65	122.60
1	A	124	ARG	NE-CZ-NH2	8.02	126.42	119.20
1	A	21	LYS	O-C-N	-7.87	111.59	122.46
1	A	88	PRO	O-C-N	-7.86	113.51	123.03
1	A	196	GLU	O-C-N	-7.84	113.81	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	193	PRO	CA-C-O	-7.66	112.38	121.95
1	A	145	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	A	194	ASN	CA-C-N	7.51	129.59	120.13
1	A	194	ASN	C-N-CA	7.51	129.59	120.13
1	A	76	VAL	N-CA-C	7.49	118.02	110.23
1	A	113	LEU	CA-C-O	7.30	128.25	120.36
1	A	48	ILE	CA-C-N	7.27	133.94	122.74
1	A	48	ILE	C-N-CA	7.27	133.94	122.74
1	A	172	GLU	CG-CD-OE2	7.27	135.12	118.40
1	A	8	CYS	N-CA-CB	7.26	121.85	111.25
1	A	183	ILE	O-C-N	-7.19	114.86	121.91
1	A	75	GLN	CA-C-O	-7.11	111.38	119.41
1	A	115	MET	CB-CA-C	7.08	123.28	109.33
1	A	267	ARG	NE-CZ-NH2	6.96	125.47	119.20
1	A	146	ASP	O-C-N	-6.90	114.03	122.25
1	A	188	ALA	O-C-N	6.83	129.47	122.09
1	A	237	ALA	CA-C-O	6.82	127.77	119.31
1	A	184	ASN	O-C-N	6.74	125.71	120.38
1	A	188	ALA	CA-C-O	-6.71	113.79	120.70
1	A	76	VAL	CA-C-O	-6.62	114.52	121.41
1	A	124	ARG	CD-NE-CZ	6.56	133.58	124.40
1	A	161	PRO	O-C-N	-6.51	114.72	122.99
1	A	144	GLN	CA-C-O	6.43	127.36	120.10
1	A	235	ILE	O-C-N	6.39	128.33	121.87
1	A	190	TRP	CA-C-N	6.39	133.74	121.54
1	A	190	TRP	C-N-CA	6.39	133.74	121.54
1	A	111	GLN	O-C-N	-6.36	114.41	121.66
1	A	9	GLY	CA-C-O	-6.18	115.21	121.64
1	A	280	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	A	287	ARG	CA-CB-CG	6.14	126.38	114.10
1	A	146	ASP	CA-C-O	6.13	126.82	119.59
1	A	88	PRO	CA-C-O	6.01	128.19	121.34
1	A	235	ILE	CA-CB-CG2	6.00	120.69	110.50
1	A	228	ARG	NH1-CZ-NH2	-5.98	111.53	119.30
1	A	19	LEU	O-C-N	5.89	128.86	122.15
1	A	183	ILE	N-CA-C	5.80	115.99	110.42
1	A	124	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	A	108	ASN	CA-CB-CG	-5.75	106.84	112.60
1	A	194	ASN	N-CA-C	5.75	118.28	111.33
1	A	111	GLN	CA-C-N	5.74	126.02	119.83
1	A	111	GLN	C-N-CA	5.74	126.02	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	GLN	CA-C-O	5.71	127.49	120.87
1	A	75	GLN	OE1-CD-NE2	-5.67	116.94	122.60
1	A	69	VAL	O-C-N	5.58	129.04	123.18
1	A	191	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	90	THR	N-CA-CB	-5.58	103.18	110.88
1	A	9	GLY	CA-C-N	-5.57	113.20	120.44
1	A	9	GLY	C-N-CA	-5.57	113.20	120.44
1	A	235	ILE	N-CA-C	5.50	117.93	111.05
1	A	163	VAL	CA-C-O	-5.50	114.51	120.67
1	A	235	ILE	CA-C-N	5.49	128.09	120.29
1	A	235	ILE	C-N-CA	5.49	128.09	120.29
1	A	102	THR	N-CA-C	-5.44	105.78	112.90
1	A	63	THR	CA-C-O	5.42	126.51	119.95
1	A	254	HIS	CA-C-O	-5.36	115.87	121.55
1	A	68	LEU	CA-C-O	-5.35	114.64	120.36
1	A	114	LEU	O-C-N	5.31	129.77	123.24
1	A	57	ASP	CA-C-N	5.30	125.11	119.28
1	A	57	ASP	C-N-CA	5.30	125.11	119.28
1	A	172	GLU	OE1-CD-OE2	-5.29	110.20	122.90
1	A	228	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	198	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	261	ASN	CA-C-O	-5.19	112.88	119.31
1	A	27	GLN	CA-C-N	-5.18	116.25	122.16
1	A	27	GLN	C-N-CA	-5.18	116.25	122.16
1	A	2	LYS	CA-C-N	-5.15	115.83	122.99
1	A	2	LYS	C-N-CA	-5.15	115.83	122.99
1	A	237	ALA	O-C-N	-5.15	115.36	122.46
1	A	15	TRP	N-CA-C	5.14	116.97	111.36
1	A	253	ARG	N-CA-C	-5.09	102.53	110.42
1	A	112	PRO	CA-C-O	-5.08	115.79	121.23
1	A	113	LEU	O-C-N	-5.08	117.26	123.30
1	A	39	VAL	CA-C-O	5.07	126.43	120.71
1	A	85	SER	O-C-N	-5.05	115.49	122.46
1	A	133	ALA	O-C-N	5.02	129.00	123.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ILE	Mainchain
1	A	75	GLN	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2256	42	0
2	A	265	0	0	10	0
All	All	2532	0	2256	42	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:CYS:HB2	2:A:477:HOH:O	1.69	0.92
1:A:205:MET:HE3	1:A:228:ARG:HB2	1.65	0.79
1:A:290:SER:O	1:A:291:GLU:HB2	1.89	0.72
1:A:198:ARG:HA	1:A:232:MET:HE1	1.74	0.69
1:A:20:CYS:SG	2:A:487:HOH:O	2.52	0.67
1:A:138:HIS:CD2	1:A:166:HIS:HE1	2.14	0.65
1:A:115:MET:HG2	1:A:169:ILE:HG21	1.81	0.62
1:A:20:CYS:HB3	2:A:487:HOH:O	2.01	0.61
1:A:138:HIS:HD2	1:A:166:HIS:HE1	1.49	0.60
1:A:104:GLU:N	1:A:104:GLU:OE2	2.35	0.57
1:A:205:MET:HE2	1:A:205:MET:HA	1.86	0.57
1:A:280:ARG:O	1:A:284:MET:HG3	2.05	0.56
1:A:189:ILE:HA	1:A:288:LYS:HE3	1.87	0.56
1:A:120:HIS:HD2	1:A:131:HIS:NE2	2.03	0.56
1:A:269:ARG:HG2	1:A:269:ARG:HH11	1.71	0.55
1:A:138:HIS:CD2	1:A:166:HIS:CE1	2.96	0.54
1:A:195:GLY:O	1:A:198:ARG:HG2	2.08	0.54
1:A:248:ASP:OD1	1:A:253:ARG:NH1	2.39	0.53
1:A:205:MET:CE	1:A:228:ARG:HB2	2.37	0.52
1:A:275:VAL:O	1:A:279:THR:HG23	2.10	0.52
1:A:141:PRO:HD3	1:A:165:TRP:CZ2	2.45	0.51
1:A:205:MET:HE3	1:A:228:ARG:CB	2.39	0.50
1:A:265:LEU:HD13	1:A:279:THR:HG22	1.95	0.49
1:A:20:CYS:CB	2:A:487:HOH:O	2.58	0.49
1:A:103:ILE:HG12	1:A:115:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:CYS:SG	1:A:26:VAL:HG21	2.54	0.47
1:A:284:MET:HE2	1:A:284:MET:HB3	1.67	0.47
1:A:194:ASN:O	1:A:235:ILE:HG23	2.15	0.47
1:A:269:ARG:HG2	2:A:553:HOH:O	2.15	0.46
1:A:176:LYS:HD3	2:A:503:HOH:O	2.16	0.46
1:A:97:HIS:HD2	1:A:98:ASN:O	1.99	0.45
1:A:177:LEU:C	1:A:177:LEU:HD23	2.41	0.45
1:A:89:VAL:HG22	1:A:89:VAL:O	2.17	0.45
1:A:72:LYS:HE3	2:A:372:HOH:O	2.17	0.45
1:A:205:MET:HE2	1:A:208:CYS:HB2	1.99	0.44
1:A:210:GLU:HB3	1:A:275:VAL:HG12	2.00	0.43
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.85	0.43
1:A:85:SER:HB3	2:A:322:HOH:O	2.17	0.42
1:A:125:ASP:HB2	2:A:496:HOH:O	2.19	0.42
1:A:196:GLU:OE2	1:A:200:HIS:HE1	2.02	0.42
1:A:269:ARG:HD2	1:A:269:ARG:HA	1.87	0.41
1:A:145:GLN:HG3	2:A:426:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/291 (99%)	284 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	247/249 (99%)	241 (98%)	6 (2%)	43 26

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	CYS
1	A	50	ASN
1	A	205	MET
1	A	209	GLU
1	A	223	SER
1	A	291	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	40	ASN
1	A	50	ASN
1	A	97	HIS
1	A	120	HIS
1	A	138	HIS
1	A	166	HIS
1	A	167	ASN
1	A	168	ASN
1	A	200	HIS
1	A	241	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.